3-(3,4-Dimethoxyphenyl)-propionic acid

Other names: Benzenepropanoic acid, 3,4-dimethoxy-
3-(3,4-Dimethoxyphenyl)propanoic acid
Inchi: InChI=1S/C11H14O4/c1-14-9-5-3-8(4-6-11(12)13)7-10(9)15-2/h3,5,7H,4,6H2,1-2H3,(H,1
InchiKey: LHHKQWQTBCTDQM-UHFFFAOYSA-N
Formula: C11H14O4
SMILES: COc1ccc(CCC(=O)O)cc1OC
Mol. weight [g/mol]: 210.23
CAS: 2107-70-2

Physical Properties

Property code	Value	Unit	Source
gf	-340.85	kJ/mol	Joback Method
hf	-586.03	kJ/mol	Joback Method
hfus	25.57	kJ/mol	Joback Method
hsub	143.60 ± 2.20	kJ/mol	NIST Webbook
hvap	71.92	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.721		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
tb	678.61	K	Joback Method
tc	875.09	K	Joback Method
tf	420.40	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.32	J/mol×K	875.09	Joback Method
cpg	422.40	J/mol×K	678.61	Joback Method
cpg	433.78	J/mol×K	711.36	Joback Method
cpg	444.55	J/mol×K	744.10	Joback Method
cpg	454.68	J/mol×K	776.85	Joback Method
cpg	464.20	J/mol×K	809.60	Joback Method

cpg	473.08	J/mol×K	842.34	Joback Method
dvisc	0.0000411	Pa×s	678.61	Joback Method
dvisc	0.0009642	Pa×s	420.40	Joback Method
dvisc	0.0004463	Pa×s	463.44	Joback Method
dvisc	0.0002355	Pa×s	506.47	Joback Method
dvisc	0.0001373	Pa×s	549.50	Joback Method
dvisc	0.0000866	Pa×s	592.54	Joback Method
dvisc	0.0000582	Pa×s	635.58	Joback Method
hfust	32.38	kJ/mol	370.90	NIST Webbook
hsubt	140.30 ± 0.80	kJ/mol	359.00	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2107702&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume